1H-Pyrrole, 1-methyl-

Other names:	1-METHYL PYRROLE
	1-Methyl-1H-pyrrole
	1-Methylpyrrol
	1-Methylpyrrole
	N-Methylpyrrol
	N-Methylpyrrole
	Pyrrole, 1-methyl-
Inchi:	InChI=1S/C5H7N/c1-6-4-2-3-5-6/h2-5H,1H3
InchiKey:	OXHNLMTVIGZXSG-UHFFFAOYSA-N
Formula:	C5H7N
SMILES:	Cn1cccc1
Mol. weight [g/mol]:	81.12
CAS:	96-54-8

Physical Properties

Property code	Value	Unit	Source
af	0.3110		KDB
chl	-3030.30 ± 0.42	kJ/mol	NIST Webbook
hf	103.10 ± 0.54	kJ/mol	NIST Webbook
hfl	62.38 ± 0.50	kJ/mol	NIST Webbook
hvap	44.60 ± 0.02	kJ/mol	NIST Webbook
hvap	40.80 ± 0.20	kJ/mol	NIST Webbook
hvap	40.70	kJ/mol	NIST Webbook
ie	7.99 ± 0.07	eV	NIST Webbook
ie	7.95 ± 0.05	eV	NIST Webbook
ie	7.94 ± 0.02	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.09 ± 0.01	eV	NIST Webbook
log10ws	-2.76		Crippen Method
logp	1.025		Crippen Method
mcvol	71.830	ml/mol	McGowan Method
pc	4850.00	kPa	KDB
rinpol	750.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	737.00		NIST Webbook

rinpol	750.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	741.00	NIST Webbook
rinpol	742.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	716.00	NIST Webbook
rinpol	731.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	735.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	738.00	NIST Webbook
rinpol	737.00	NIST Webbook
rinpol	722.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	722.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	717.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	717.00	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	741.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	730.00	NIST Webbook
rinpol	719.00	NIST Webbook
rinpol	717.00	NIST Webbook
rinpol	725.00	NIST Webbook
rinpol	739.00	NIST Webbook
rinpol	715.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	702.00	NIST Webbook
rinpol	710.00	NIST Webbook
rinpol	731.00	NIST Webbook
rinpol	710.00	NIST Webbook
rinpol	731.00	NIST Webbook
ripol	1180.00	NIST Webbook
ripol	1154.00	NIST Webbook
ripol	1148.00	NIST Webbook

ripol	1140.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1155.00		NIST Webbook
ripol	1137.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1129.00		NIST Webbook
ripol	1157.00		NIST Webbook
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ripol	1168.00		NIST Webbook
ripol	1157.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1127.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1140.00		NIST Webbook
ripol	1147.00		NIST Webbook
ripol	1139.00		NIST Webbook
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ripol	1144.00		NIST Webbook
ripol	1139.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1139.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1166.00		NIST Webbook
ripol	1171.00		NIST Webbook
ripol	1195.00		NIST Webbook
ripol	1170.00		NIST Webbook
sl	200.52	J/mol×K	NIST Webbook
sl	200.48	J/mol×K	NIST Webbook
sl	200.48	J/mol×K	NIST Webbook
tb	385.80	K	KDB
tc	597.00	K	Thermodynamic properties of pyrrole, 1-methylpyrrole, 2,4-dimethylpyrrole, and 2,5-dimethylpyrrole: Experimental and computational results
tc	596.00	K	KDB
tf	322.11	K	KDB
tf	231.20 ± 0.50	K	NIST Webbook

tf	216.82 ± 0.08	K	NIST Webbook
tf	216.91	K	NIST Webbook
tt	216.87 ± 0.01	K	NIST Webbook
tt	216.91 ± 0.03	K	NIST Webbook
tt	216.91 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	150.06	J/mol×K	298.15	NIST Webbook
cpl	150.06	J/mol×K	298.15	NIST Webbook
cpl	150.06	J/mol×K	298.15	NIST Webbook
hfust	7.82	kJ/mol	216.91	NIST Webbook
hfust	7.82	kJ/mol	216.91	NIST Webbook
hfust	7.82	kJ/mol	216.90	NIST Webbook
hfust	7.82	kJ/mol	216.90	NIST Webbook
hvapt	39.00	kJ/mol	372.00	NIST Webbook
hvapt	38.00	kJ/mol	353.00	NIST Webbook
sfust	36.07	J/mol×K	216.91	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40817e+01
Coeff. B	-3.09648e+03
Coeff. C	-5.87940e+01
Temperature range (K), min.	283.27
Temperature range (K), max.	411.86

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.94030e+01
Coeff. B	-7.46125e+03
Coeff. C	-9.43097e+00

Coeff. D	4.78467e-06
Temperature range (K), min.	216.91
Temperature range (K), max.	610.00

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of pyrrole, 1-methylpyrrole, 2,4-dimethylpyrrole, and 2,5-dimethylpyrrole: Experimental and computational results:	https://www.doi.org/10.1016/j.jct.2017.09.005
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1344.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96548&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1344

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

tt: Triple Point Temperature